Materials Modeling for Superconducting Radio-Frequency (SRF) Cavities

- Niobium SRF cavities will provide the accelerating gradient for high-performance linear particle accelerators
  - International Linear Collider
  - Project X
  - External applications

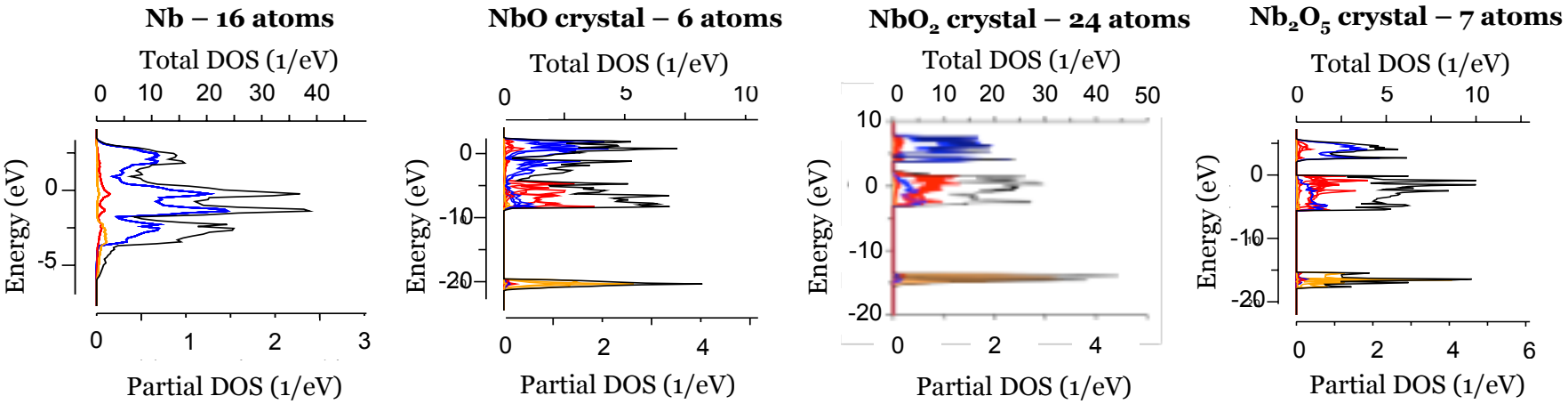
http://newsline.linearcollider.org/images/2010/20100617_dc_1.jpg

- SRF cavity forming and processing R&D is ongoing - the fundamental mechanisms of each step are not fully understood!
- SRF cavities can fail according to several mechanisms related to defects in the cavity material (e.g. surface roughness, impurity incorporation), which can result from cavity processing
- Density Functional Theory implemented in VASP on the Wilson Cluster is used to model the material science of SRF cavities on the atomic scale

Example 1: Properties of Niobium Oxides

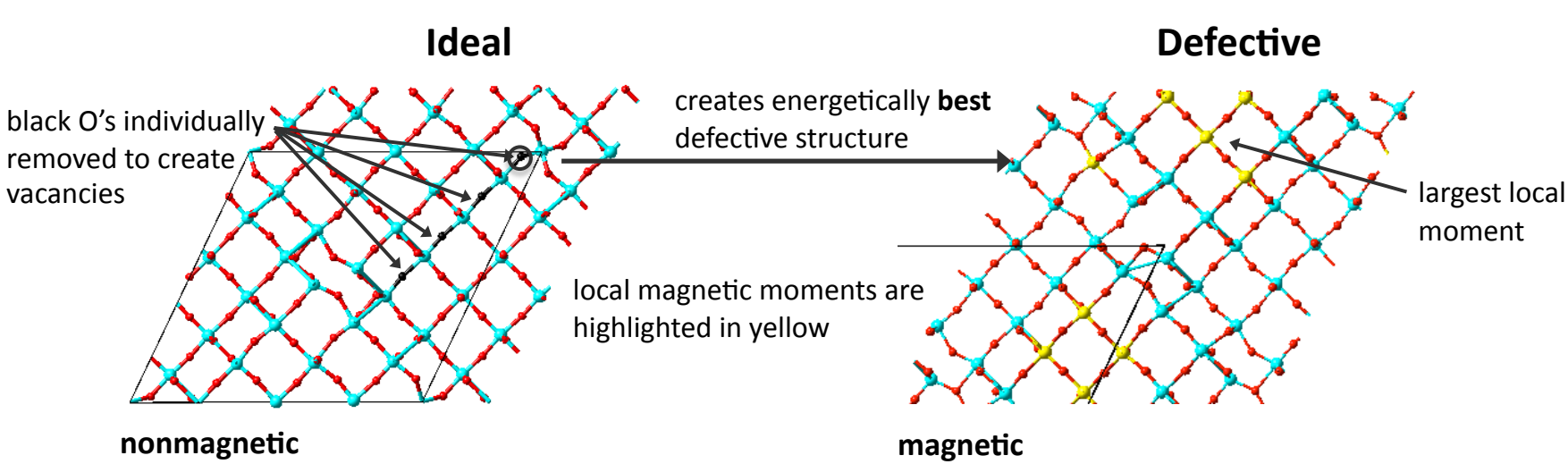
- The niobium surface is covered with an oxide layer which can be altered during several steps in the cavity processing procedure
- Oxygen content and oxide structure affect the electronic, magnetic, and superconducting properties of the the cavities

VASP Model of Ideal Structures



Example 1: Properties of Niobium Oxides

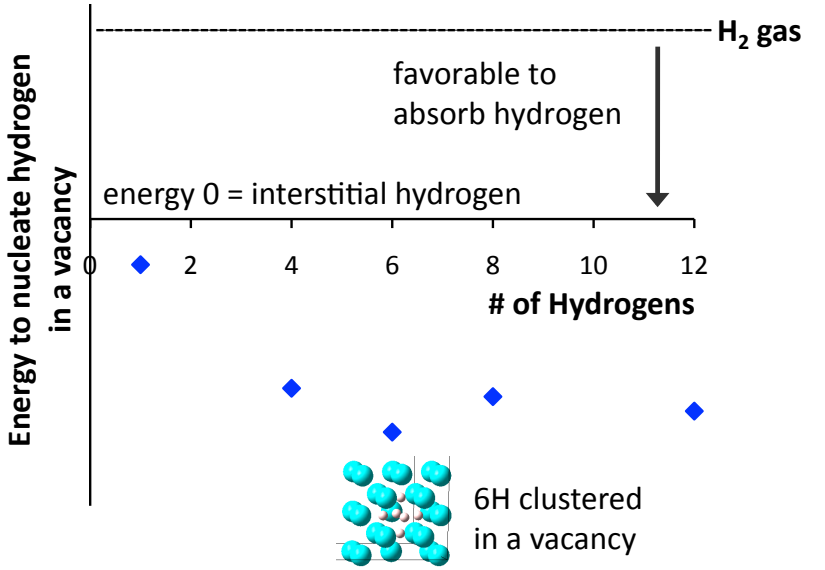
- Structural defects can affect local material properties
- Local material properties may affect cavity performance

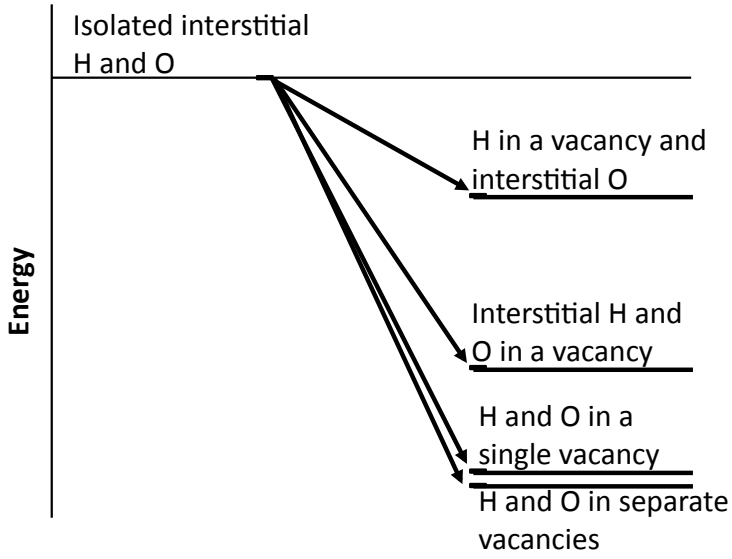


Example 2: Thermodynamic Evaluation of Impurity Attraction to Structural Defects

- Niobium can easily absorb hydrogen and oxygen
- Defects in metal structures can nucleate chemical impurities
- Precipitates may lead to degraded cavity performance

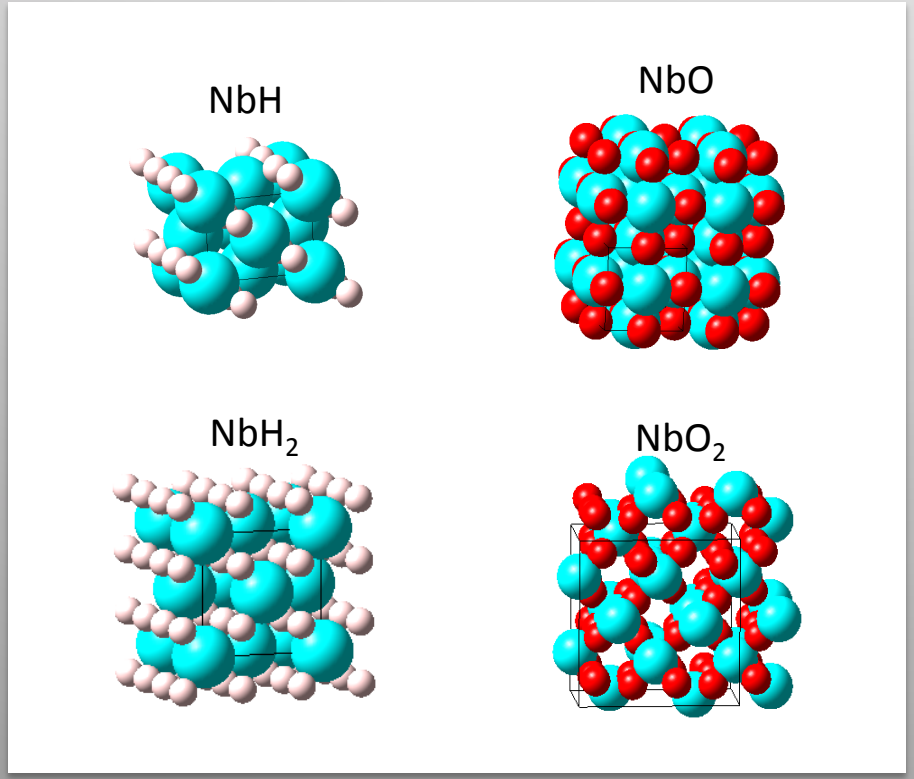
VASP Model of Impurity Attraction to Nb vacancies





Example: Construction and Evaluation of Crystal Structures

Successfully model experimentally known structures (get from ICSD – XRD)



Create and Compare Plausible Precipitate Structures